

1 *Supplementary information for*

2 **Dispersion and Dosimetric Challenges of Hydrophobic**
3 **Carbon-Based Nanoparticles in In Vitro Cellular Studies**

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19 **Summary**

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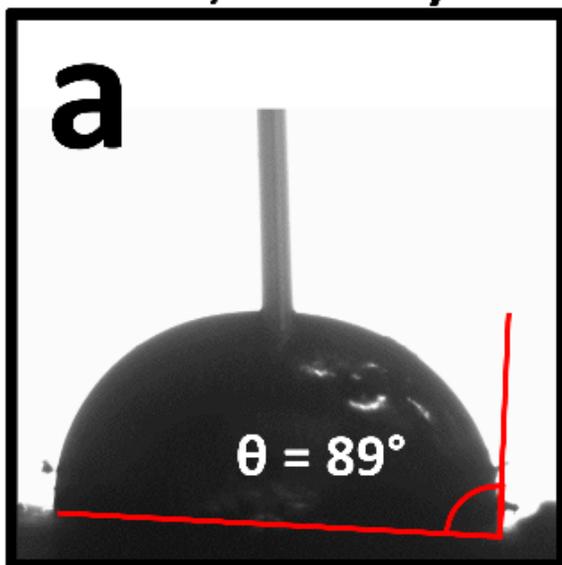
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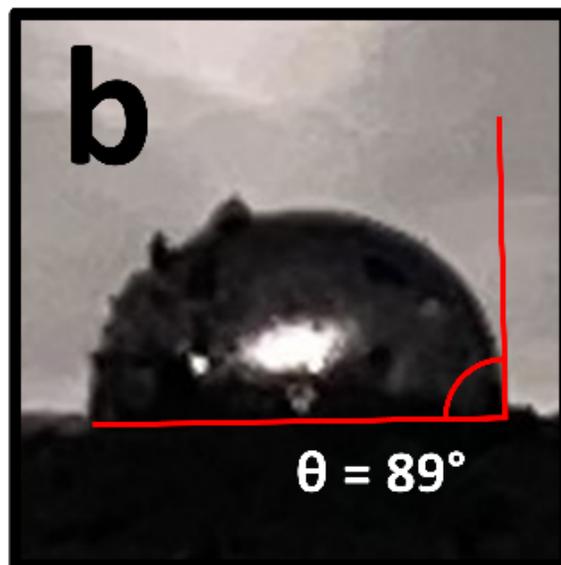
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OCA35, DataPhysics



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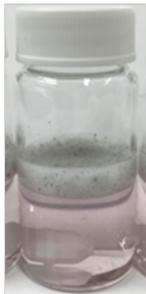
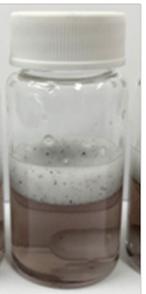
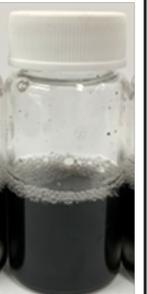
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30 **Figure S1.** Water Contact Angle (WCA) measured with a) a high precision optical measuring
31 device (OCA35, DataPhysics) and b) the custom goniometer used in this work.

32 **Table S1.** Summary of the parameters used for the particle dosimetry calculation by the DG model.
 33 The viscosities of the media were measured by a Cannon Fenske viscometer for water-based
 34 solutions, submerged in a heating bath equilibrated to 37 °C. The densities were measured by
 35 weighing a known volume of the medium pre-warmed to 37 °C in a heating bath.

		RPMI	SABM
Particle Parameters	Material	User defined	
	Density	1.8 g/cm ³	
	Distribution type	Fraction distribution by volume	
	Effective density	1.03 g/cm ³	1.07 g/cm ³
Solvent Parameters	Density	1.0104 g/cm ³	0.995 g/cm ³
	Viscosity	0.0081 P	0.0075 P
	Temperature	37 °C	37 °C
Simulation Parameters	Suspension column height	4.5 mm	
	Height of subcompartment	0.005 mm	
	Initial total concentration of material	0.1 mg/cm ³	
	Centrifugation	1 (gravity)	
	Total time of simulation	24 h	
	Time interval for simulation	0.5 s	
Output Parameters	Time interval	30 min	
	Compartment height	0.01 mm	
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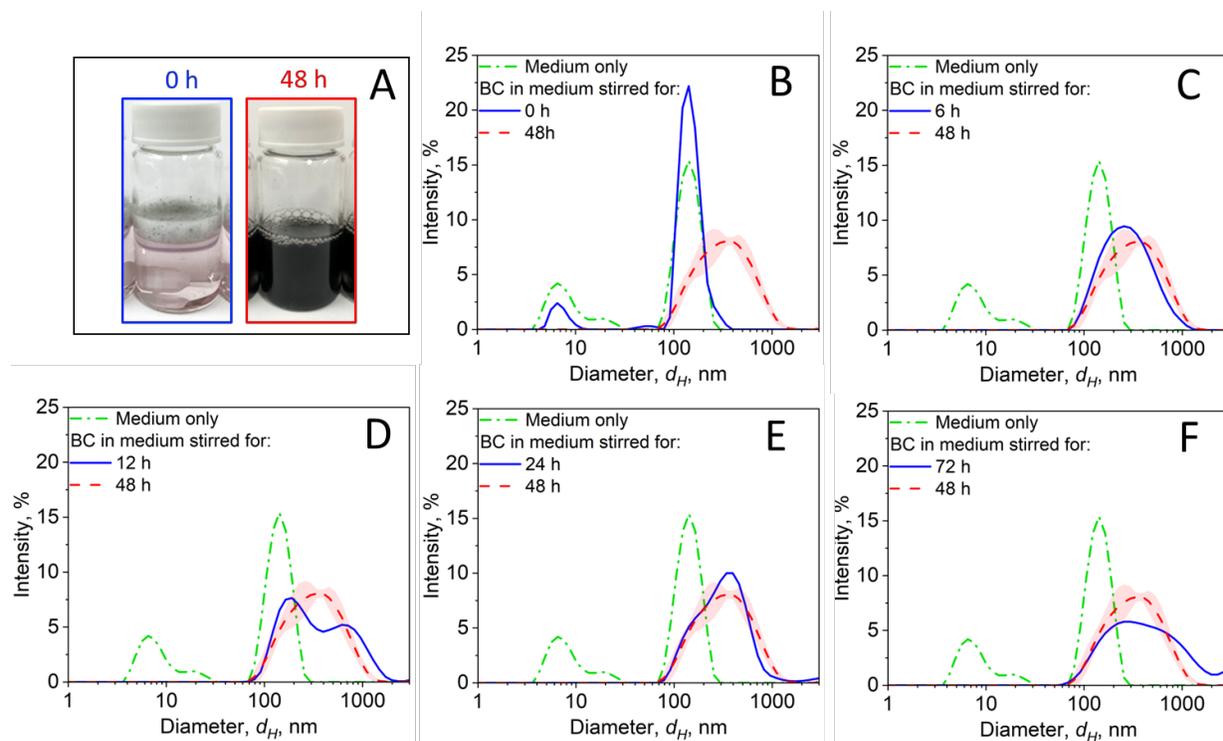
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	0 h	6 h	12 h	24 h	48 h	72 h
RPMI						
Z-Average	98 nm	347 nm	345 nm	329 nm	347 nm	331 nm
SABM						
Z-Average	218 nm	280 nm	319 nm	336 nm	309 nm	365 nm

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38 **Figure S2.** Representative images of BC NPs dispersed in RPMI (top) and SABM (bottom) after
 39 stirring for 0-72 h along with the respective Zeta-Average (Z-Average) measured by Dynamic
 40 Light Scattering (DLS).

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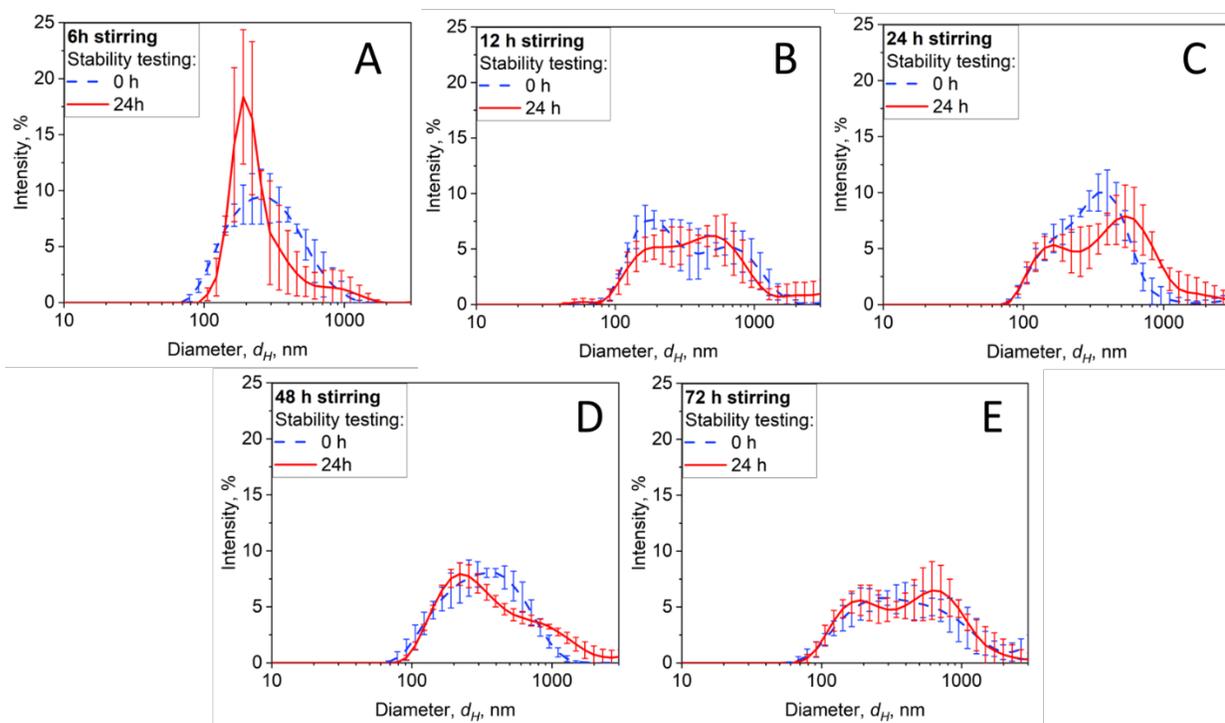


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 43 **Figure S3.** Representative images (A) of the dispersions of BC NPs in SABM medium after
 44 stirring for 0 (blue-framed) and 48 h (red-framed), along with intensity-based particle size
 45 distributions measured by DLS for the medium only (dot-broken line) or BC dispersions after 0
 46 (B), 6 (C), 12 (D), 24 (E), 72 (F) or 48 h (broken line). Variation within three DLS measurements
 47 of the sample stirred for 48 h is quantified by the red shaded area.

48
 49 **Table S2.** Zeta potential and conductivity of BC NPs dispersed in RPMI and SABM
 50 media measured by DLS for stable dispersions obtained at 24 h and 48 h of stirring, respectively.

	Zeta Potential (mV)	Conductivity (mS/cm)
BC in RPMI	-13 ± 2	15.7 ± 1.3
BC in SABM	-12 ± 1	14.2 ± 0.8

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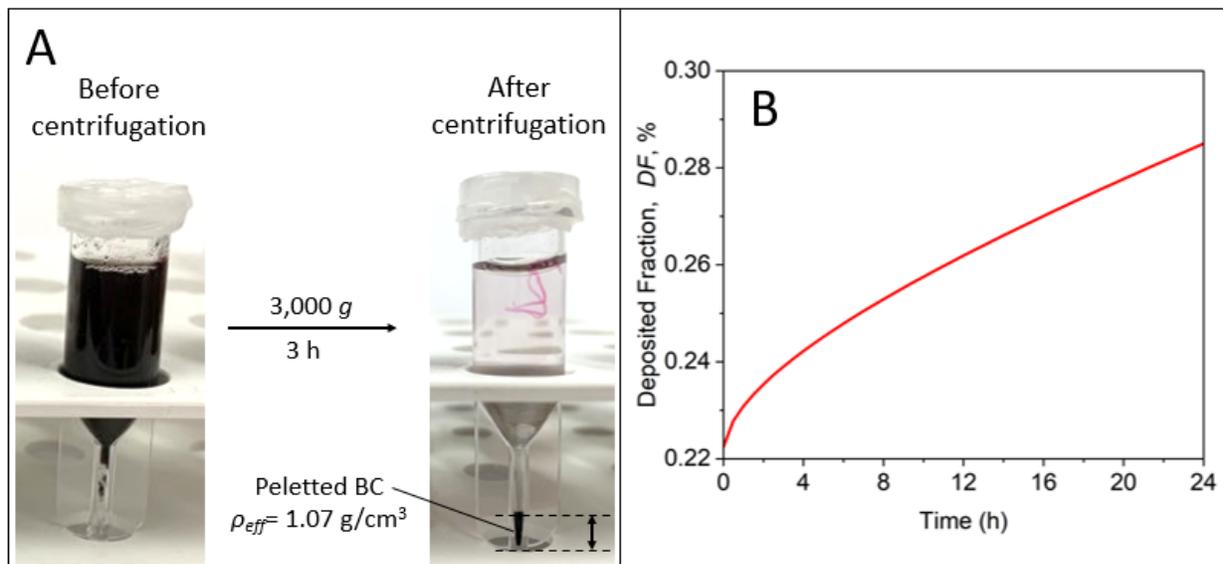
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53 **Figure S4.** Stability of the BC size distribution measured in SABM medium right after stirring
 54 (broken lines) for 6 (A), 12 (B), 24 (C), 48 (D) and 72 h (E) or after 24 h of storage at room
 55 temperature (solid lines). The errorbars quantify the statistical variation over 3 measurements.

56 **Table S3.** Z-Average and polydispersity index (PDI) of BC NPs stirred in SABM medium from
 57 the data shown in Figure S4.

BC in SABM stirred for:	Immediately after stirring		Stability testing (24 h)	
	Z-Average (nm)	PDI	Z-Average (nm)	PDI
6 h	280 ± 19	0.407 ± 0.016	321 ± 54	0.469 ± 0.051
12 h	319 ± 14	0.410 ± 0.019	415 ± 6	0.735 ± 0.037
24 h	336 ± 26	0.431 ± 0.022	326 ± 33	0.456 ± 0.064
48 h	309 ± 9	0.409 ± 0.042	334 ± 12	0.492 ± 0.044
72 h	365 ± 7	0.518 ± 0.087	379 ± 17	0.476 ± 0.052

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60 **Figure S5.** Effective density, ρ_{eff} , of BC NPs in SABM medium established by VCM method (A)
 61 and the deposited fraction calculated by the DG model (B).